PROBABILISTIC EVALUATION OF MODELS FOR THE ATMOSPHERIC DISPERSION OF EFFLUENTS RELEASED FROM A COMPLEX SITE

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INTRODUCTION

The validation and reliability of atmospheric dispersion models are important concerns for both model users and developers. Numerous field experiments have been conducted to address these issues of model reliability, with the results of the field experiments often being used to evaluate differences between the performance of different models (e.g. Hanna *et al*., 2001; Hill *et al*., 2001). However, atmospheric dispersion models have a number of sources of uncertainty. These include the errors in model formulations and model physics that will vary between models, though errors in model inputs and those due to the inherent uncertainties that are caused by stochastic atmospheric process are also considered to be important (Fox, 1984; Venkatram, 1988).

This paper develops a probabilistic modelling framework to estimate the errors in both model input data and those caused by the stochastic nature of atmospheric turbulence. This probabilistic methodology was then used to provide input data sets for a simple Gaussian plume atmospheric dispersion model. Meteorological measurements were used to assign distributions to key input parameters. Finally, the probabilistic distributions output by the model were compared with field measurement data from BNFL Sellafield (^{85}Kr air concentrations and ^{41}Ar gamma doses) to investigate the underlying causes of model uncertainty found in previous validation studies conducted by Hill *et al*. (2001) and Lowles *et al*. (2001).

ATMOSPHERIC DISPERSION MODELLING

The R91 Gaussian plume atmospheric dispersion model (Clarke, 1979) was used in this study. This model uses the Pasquill-Gifford stability classification scheme to subdivide atmospheric stabilities into seven types ranging from A (highly unstable) to G (highly stable). The model does not account for variations in plume spread with height in the atmosphere, though the relationship between plume advection speed and height was approximated through the use of a simple power law relationship.

The R91 model was selected based on its simplicity and speed, enabling the model to be run with more that 2,500 Monte Carlo sampled input parameter sets per hour of meteorological data. Also, field validation experiments have shown that the performance of the R91 model is similar to that of the more complex UKADMS model when both models are run using effective stack heights determined from wind tunnel studies. Further details of the modelling methods used and the results of the intercomparisons between R91 and UK-ADMS can be found in Hill *et al*. (2001) and Lowles *et al*. (2001).

DEVELOPMENT OF A MONTE CARLO MODEL

Monte Carlo techniques have been extensively used to evaluate the uncertainty in atmospheric dispersion models. However, it is important to recognise that the methods are limited by the realism and generality of the input distributions that are used. The Monte Carlo model that was developed in this study had to utilise uncertainty distributions for the input data required by the

R91 dispersion model. These fall into three generic groups: (i) receptor data; (ii) source data and (iii) meteorological data.

The development of a Monte Carlo model was straightforward for groups (i) and (ii) as the model input data could be directly assigned probability distributions that were independent of the other sources of uncertainty in the model. The uncertainties in the bearing and distance to the receptor location were both estimated to be normally distributed with a standard deviation of 5^o and 5% of the best estimate value respectively for distances less than 1.5 km. The source emission data uncertainties, were included as normal distributions with standard deviations of +/- 5 % of the emission rate for all sources. This approximation was based on calibration data supplied by the Sellafield site. The uncertainties in the effective stack heights were determined directly from the original wind tunnel studies and were included in the model as uniform distributions ranging from 58-80m and 75-95m for the two stacks that discharge ^{85}Kr and from 15-40m for each of the reactor stacks that discharge ^{41}Ar.

A meteorological module was developed to account for the correlated uncertainties in hourly meteorological input data (group iii), as shown in Figure 1. As the underlying cause of the correlations between meteorological uncertainties was the intensity of atmospheric turbulence (which is itself related to the wind speed) a feedback loop was included enabling the uncertainty distributions of the wind speed, wind direction and standard deviation of the wind direction (termed sigma-theta) to vary with wind speed.

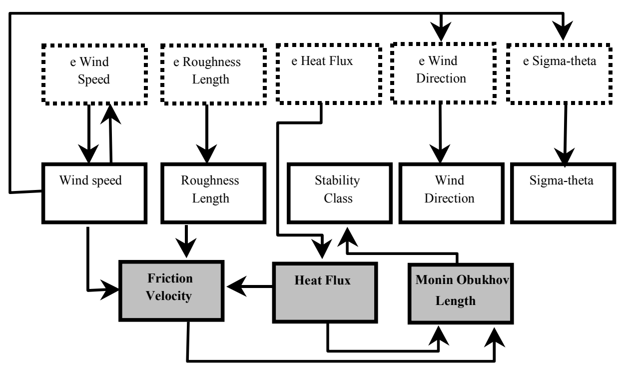

Figure 1: Detailed structure of the meteorological module of the Monte Carlo model. Boxes with a dashed outline indicate uncertainty distributions (e) from which model input data (solid line) were determined. The shaded boxes are calculation modules and were not directly input to the R91 model.

A further consideration when developing the meteorological module was the calculation of the uncertainty in the stability class. This could not simply be assigned a distribution and consequently was calculated from the relationship between Monin-Obukhov length and stability class derived by Golder (1972). This was achieved by including the surface heat flux (and its uncertainty distribution) as an input to the Monte Carlo model. An iterative technique was used to determine friction velocities and Monin-Obukhov lengths from wind speed and heat flux data. Uncertainties in wind speeds, wind directions and sigma-theta values were estimated by analysing paired wind speed and wind direction readings collected from opposite sides of the BNFL Sellafield site. The use of this experimental dataset allowed the uncertainty model to capture both the instrument error and the stochastic uncertainty in meteorological measurements. For wind speed and sigma-theta data the hourly co-efficient of variation (CV) corresponding to each time period that measurements were recorded was calculated from the paired measurements (termed *d1* and *d2*) using equation 1, where σ is the standard deviation. For wind direction data the difference in angle between the paired measurements was calculated.

$$CV = \frac{\sigma\{d1, d2\}}{0.5(d1 + d2)} \quad (1)$$

Data were subdivided into nine wind speed ranges with the limits to these ranges calculated by ensuring that each range contained approximately the same number of data points (approximately 350 hours). A median value of either CV or wind direction difference was evaluated as the "best estimate" of the uncertainty within each of the ranges. The results of this analysis are shown in Table 1. All the distributions were parameterised in the model using normal distributions with the mean being given by each hours deterministic measurement from the Sellafield meteorological station. The standard deviations of the distributions for wind speed and sigma-theta were calculated from the median CV values, whilst the standard deviation for the wind direction was taken directly from the median wind angle difference.

Table 1. Analysis of the uncertainty in meteorological data determined from paired meteorological measurements.

Wind Speed bin ($m\ s^{-1}$)	Median CV Wind Speed (non dimensional)	Median CV Sigma-theta (non dimensional)	Median Wind Angle Difference (degrees)
<1.9	0.19	0.55	31.75
>1.9 <2.5	0.17	0.57	22.15
>2.5 < 3.2	0.13	0.49	14.62
>3.2 <4.1	0.12	0.40	10.04
>4.1 <5.0	0.13	0.36	5.93
>5.0 <6.0	0.14	0.31	5.32
>6.0 <6.9	0.15	0.35	5.35
>6.9 <8.1	0.16	0.36	5.52
>8.1	0.15	0.32	5.27

The uncertainty in the heat flux was determined from paired eddy correlation and flux profile measurements collected at the meteorological site. The standard deviation of the heat flux was estimated to be +/- 40% of the mean value and a normal distribution was used to include this error term in the Monte Carlo model.

COMPARISON BETWEEN FIELD MEASUREMENTS AND PROBABILISTIC MODELLING

Data within the ^{85}Kr and ^{41}Ar field measurement databases were compared with the predictions of the R91 model run using probabilistic input data. Data were selected from the ^{41}Ar monitoring database for periods of 1 hour and 24 hours when the gamma doses were above the limit of detection of 1 $nSv\ hr^{-1}$. These data relate to dispersion from the Calder reactors to the critical group. Data were selected from the ^{85}Kr database for monitoring periods when receptor locations were within 1.5 km of the site, averaging times were between 2-48 hours and air concentrations were above 5 $Bq\ m^{-3}$.

The field measurements were compared with these distributions to assess the probability that the model would predict the value measured in the field. Due to the bias (an overprediction by the model) identified between the ^{85}Kr measurements and the model predictions in Hill *et al*. (2001) a simple correction factor (a factor of 2.0) was applied to account for what appears to be an error in the model formulation or physics. Corrected and uncorrected data were both included in the subsequent analysis. A summary of these input data and the percentage of the measurements that were within the range of the probabilistic model are shown in table 2.

Table 2: Comparison of selected data from the ^{85}Kr and ^{41}Ar databases with the range of predictions from the probabilistic Monte Carlo model.

	^{85}Kr Air Concentrations		^{41}Ar Gamma Doses	
	Uncorrected	Bias corrected	Hourly	Daily
Number of measurements	88	88	938	47
Measurements ranking within the 0-100 percentiles of the model range	90%	92%	96%	92%

The data shown in Table 2 illustrate that the probabilistic model had performed well and accounted for the differences between the model predictions and the field measurements for more than 90% of the data that were evaluated. It was particularly encouraging that the model described the variation in the ^{41}Ar measurements collected over both 1 and 24 hour averaging periods as this illustrates the generality of the uncertainty model.

It was also important to establish how well the uncertainty model described the range of variability that was found between model predictions and the field measurements. This was in order to establish that the uncertainty model had not grossly overestimated the range that concentrations or doses could take. If the probabilistic model had accounted for all sources of model uncertainty then the field measurements would sit at random positions across the entire probabilistic range.

The above test was applied to the Monte Carlo model by evaluating the percentile that each of the field measurements was located on the corresponding modelled probabilistic range. This process was repeated for all the data selected from the ^{85}Kr and ^{41}Ar databases. In order to convert from continuous probabilities to discreet probabilities the percentiles were binned into 10 categories. A graph of these distributions is shown in Figure 2.

The data shown in Figure 2 demonstrate that the combined Monte Carlo/atmospheric dispersion model did not sample uniformly across all percentile bins, with chi-squared tests confirming that there were significant differences between the model predictions and homogeneity. In general though, the model was found to realistically represent the range of values from the field datasets, indicating that much of the variability found in the previous validation studies was due to input data errors and stochastic variations in meteorological data. The differences shown in figure 2 could be reduced by using a more sophisticated dispersion model (particularly the over predictions of low percentile ranges for the ^{85}Kr measurements), by refinement of the parameters used in the Monte Carlo model or by evaluating a larger set of measurements.

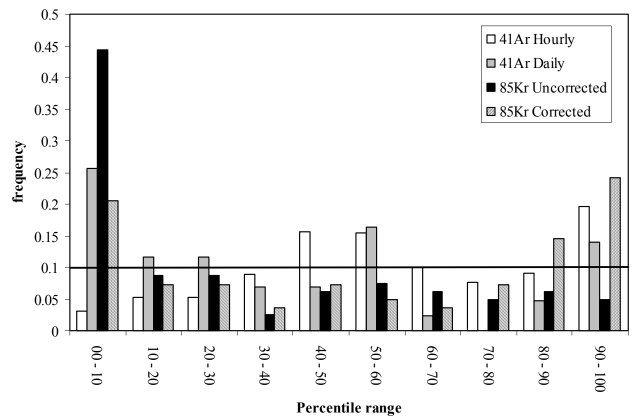

Figure 2: Probability distribution showing the frequency that each of 10 percentile ranges of the Monte Carlo uncertainty model were represented by field measurements from the ^{85}Kr and ^{41}Ar databases. The horizontal line shows the results that would be expected from a perfect model.

CONCLUSIONS

A probabilistic Monte Carlo modelling methodology, accounting for uncertainties in receptor data, source data and meteorological data, was developed and applied as a pre-processor to the simple R91 atmospheric dispersion model. The probabilistic predictions of the R91 model were compared with extensive field datasets of ^{85}Kr air concentrations and ^{41}Ar gamma doses. The results of this comparison showed that the probabilistic model accounted for a high proportion of the uncertainty found in the field measurements, indicating that uncertainties in model inputs and due to the stochastic nature of turbulence predominate. Further model intercomparison studies could use similar techniques to assess the uncertainties that result from differences in model formulations.

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